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PHYSICS LETTERS A

Physics Letters A 371 (2007) 1–6

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Plasmon dispersion in metallic carbon nanotubes in the presence of low-frequency electromagnetic radiation

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Received 15 March 2007; received in revised form 17 May 2007; accepted 22 May 2007

Available online 9 June 2007

Communicated by C.R. Doering

Abstract

We present theoretical analysis of plasmon dispersion in two-walled metallic carbon nanotubes in the presence of low-frequency electromagnetic radiation, based on classical electrodynamic formulations and linearized hydrodynamic model of carbon valence electrons. Calculations are performed for the transverse magnetic and transverse electric waves, respectively, by solving Maxwell and hydrodynamic equations with appropriate boundary conditions.

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PACS: 41.20.Jb; 73.22.Lp; 42.25.Bs

Keywords: Carbon nanotubes; Electromagnetic wave; TM mode; TE mode; Plasmon dispersion

1. Introduction

Since the discovery of carbon nanotubes by Iijima [\[1\],](#page--1-0) a lot of experimental [\[2–5\]](#page--1-0) and theoretical [\[6–19\]](#page--1-0) work has been done to study the collective electronic excitations in these systems. Lin and Shung [\[6\]](#page--1-0) evaluated the dielectric function within the random phase approximation (RPA), the zeros of this function define the plasmon modes. They have found uncoupled acoustic and optical plasmon branches for zero and nonzero angular momentum changes, respectively. In their recent paper Lin and Shyu [\[7\]](#page--1-0) replaced the two-dimensional confinement by a tight-binding model but only for the π electrons and described low-frequency electronic excitations in carbon nanotubes, then Ho et al. [\[8\]](#page--1-0) studied the effects of the intertube atomic overlaps and the intertube Coulomb interactions on low-frequency electronic excitation in two-walled armchair carbon nanotubes (2WNT). Longe and Bose [\[9\]](#page--1-0) used the two-dimensional model with the (RPA) for single-walled nanotubes (SWNT) and a classical dynamical model for multi-walled nanotubes (MWNT) to calculate the dielectric function and the dispersion relations for the collective oscillations and found one acoustic and several optical branches. The calculation of plasmon dispersion in a MWNTs was first presented in [\[9\].](#page--1-0) With a classical hydrodynamic model, Yannouleas et al. [\[10\]](#page--1-0) and Jiang [\[11\]](#page--1-0) studied the collective excitation behaviours of *σ* and *π* electrons for single and multi-walled nanotubes. Recently, Perez and Que [\[12\]](#page--1-0) showed that the plasmon dispersions can depend strongly on the chirality of carbon nanotubes. The non-dispersive modes could be due to chiral nanotubes, and the dispersive mode should be due to armchair and zigzag nanotubes. In Fig. 2 of that paper, one can see that the (16, 3) tube has only optical modes, while the (10, 10) and (18, 0) tubes each have an acoustic mode. This is because the (16, 3) tube is semiconducting while the other tubes are metallic. The plasmon modes are localized collective electronic oscillations that can be excited by charged particles or electromagnetic radiation. Mowbray et al. with hydrodynamic model, studied interactions of fast charged particle with carbon nanotubes and calculated the

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^{0375-9601/\$ –} see front matter © 2007 Elsevier B.V. All rights reserved. [doi:10.1016/j.physleta.2007.05.110](http://dx.doi.org/10.1016/j.physleta.2007.05.110)

plasmon dispersion for a SWNT using the two fluid model [\[13\]](#page--1-0) and a 2WNT using a single fluid model [\[14\],](#page--1-0) then Chung et al. [\[15\]](#page--1-0) planed on calculating the plasmon energies for a MWNT using the two fluid model. In recent studies of electromagnetic wave propagation in SWNT [\[16\],](#page--1-0) it has been shown that dispersion behaviours of the TE and TM modes are quite similar and dispersion relation of the two types of modes are similar with that of the well-known electrostatic collective excitations [\[10\],](#page--1-0) which has a dimensionality crossover from a 1D system to a 2D system. For 2WNT the coupling between the two layers leads to important modifications. In the present work, based on a linearized hydrodynamic theory and classical electrodynamic formulations, we show that the plasmon dispersion in metallic 2WNT can be obtained in the presence of low-frequency electromagnetic radiation with transverse magnetic and transverse electric modes.

2. Formulation of the problem

We consider a infinitely long and infinitesimally thin 2WNT, with radii $a_1 < a_2$. Let us assume that the density of free-electron fluid over the each cylindrical surface (per unit area) is $n_0 = 4 \times 38$ nm⁻², corresponding to four valence electrons per carbon atom. We use cylindrical coordinates $\mathbf{x} = (r, \phi, z)$ for an arbitrary point in space, and define $\mathbf{x}_i = (a_i, \phi, z)$ to represent the coordinates of a point on the cylindrical surface $r = a_j$ (with $j = 1, 2$). Assuming that $n_j(\mathbf{x}_j, t)$ is the perturbed density (per unit area) of the homogeneous electron fluid on the *j* th wall, due to propagation electromagnetic wave with frequency *ω*, along the nanotube axis *z*. Based on the linearized hydrodynamic model, one obtain the linearized continuity equation, for each *j* [\[17\],](#page--1-0)

$$
\frac{\partial n_j(\mathbf{x}_j, t)}{\partial t} + n_0 \nabla_j \cdot \mathbf{u}_j(\mathbf{x}_j, t) = 0,\tag{1}
$$

and the linearized momentum-balance equation,

$$
\frac{\partial \mathbf{u}_j(\mathbf{x}_j, t)}{\partial t} = -\frac{e}{m_e} \mathbf{E}(\mathbf{x}_j, t) - \frac{\alpha}{n_0} \nabla_j n_j(\mathbf{x}_j, t) + \frac{\beta}{n_0} \nabla_j \big[\nabla_j^2 n_j(\mathbf{x}_j, t) \big],\tag{2}
$$

where $\mathbf{E}(\mathbf{x}_i, t) = E_z \hat{\mathbf{e}}_z + E_\phi \hat{\mathbf{e}}_\phi$ is the tangential component of the electromagnetic field on the cylindrical surface for each *j*, *e* is the element charge, m_e is the electron mass, $\mathbf{u}_j(\mathbf{x}_j, t)$ is the velocity of the electrons residing on the *j*th shell and $\nabla_j =$ $\hat{\mathbf{e}}_z(\partial/\partial z) + a_j^{-1} \hat{\mathbf{e}}_{\phi}(\partial/\partial \phi)$ differentiates only tangentially to that surface. In the right-hand side of Eq. (2), the first term is the force on electrons due to the tangential component of the total electric field, evaluated at the nanotube surface $r = a_j$, the second and third terms arise from the internal interaction force in the electron fluid with $\alpha = v_F^2/2$ is the square of the speed of propagation of density disturbances in a uniform 2D homogeneous Thomas–Fermi electron fluid [with the Fermi speed $v_F = (2\pi n_0 a_B^2)^{1/2} v_B$] and $\beta = (a_B v_B)^2/4$. Here a_B and v_B are the Bohr radius and the Bohr velocity, respectively. The electric field vector $\mathbf{E}(\mathbf{x},t)$ and the magnetic field vector $\mathbf{B}(\mathbf{x},t)$ can be expanded in the following Fourier forms

$$
\mathbf{E}(\mathbf{x},t) = \sum_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dq \, \mathbf{E}_m(r,q) e^{i(m\phi + qz - \omega t)},\tag{3}
$$

and

$$
\mathbf{B}(\mathbf{x},t) = \sum_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dq \, \mathbf{B}_m(r,q) e^{i(m\phi + qz - \omega t)}.
$$
 (4)

From Eqs. (1) and (2) after the elimination of the velocity $\mathbf{u}_i(\mathbf{x}_i, t)$, one obtain

$$
n_j(\mathbf{x}_j, t) = \sum_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dq \, N_{jm}(q) e^{i(m\phi + qz - \omega t)}, \tag{5}
$$

where

$$
N_{jm} = -\frac{ien_0}{m_e} \frac{1}{\Omega_{jm}} \left(qE_z + \frac{m}{a_j} E_\phi \right),\tag{6}
$$

and

$$
\Omega_{jm} = \omega^2 - \alpha \left(q^2 + \frac{m^2}{a_j^2} \right) - \beta \left(q^2 + \frac{m^2}{a_j^2} \right)^2. \tag{7}
$$

By using Maxwells equations, one obtain the following Helmholtz equations for the *z*-components *Ezm* and *Bzm* of the expanding coefficients **E***zm* and **B***zm*

$$
\frac{d^2}{dr^2}\left(\frac{E_{zm}}{B_{zm}}\right) + \frac{1}{r}\frac{d}{dr}\left(\frac{E_{zm}}{B_{zm}}\right) - \left(\kappa^2 + \frac{m^2}{r^2}\right)\left(\frac{E_{zm}}{B_{zm}}\right) = 0,\tag{8}
$$

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